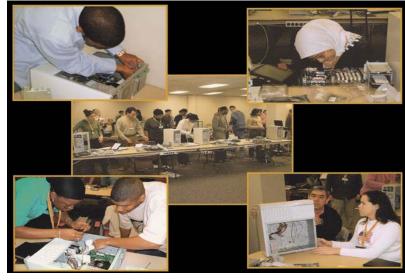
## Computational Science Workshop for Underrepresented Groups

- Annual series of workshops for undergraduate students & their faculty mentors from underrepresented groups
- Workshops provide participants
  with hands-on experience in parallel
  computing, including the assembly
  of a Linux cluster from components
- The parallel cluster is used for algorithmic & simulation exercises in a tutorial setting
- Participants also visit various research laboratories & attend lectures on emerging trends in bioinfo-nano sciences



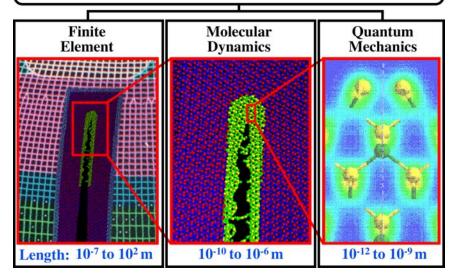
"I am one of the students who recently attended your workshop, and I was just writing to sincerely thank you for selecting me to be a part of such an astounding experience. I cannot believe how much I learned in one week, and it was so much fun. I am so glad that I attended the workshop because being in undergraduate school, I do not usually get a chance to do much hands-on work, but I mainly have to do a lot of difficult programming. At one time I was so frustrated with only having to program and not getting any hands-on experience that I almost considered changing my major. However, during the workshop I was so mesmerized by all of the hands-on experience, especially when we built the parallel computer. Your workshop helped me to remember why I wanted to be a computer science major in the first place. I feel so inspired now to go on and get my PhD in computer science. I hope that you will continue the workshop for many years so that other students will be so richly enhanced, just as the workshop enhanced me. I hope that when I obtain my PhD I will be able to return to the workshop no longer as a student but as a mentor for other students. I want to be able to help inspire others just as all of you in the workshop helped to inspire me."

Tanjala Purnell a participant at our Computational Science Workshop for Underrepresented Groups, January 5-11, 2003.

## **Multiscale Grid Simulation**

- Seamless integration of:
  - > Molecular dynamics 108-109 atoms
  - > Density functional theory 10<sup>3</sup> atoms
  - > Finite element
- Implemented on a Grid of
  4 Linux clusters in the US
  & Japan
- Studied stress corrosion of a crack in silicon by water

Seamless Multiscale Integration of Molecular Dynamics with Quantum Mechanical & Finite Element Methods



## **Grid Computing**

